

Quantum Simulation of Quantum Channels in NMR

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We propose and experimentally demonstrate an efficient framework for the quantum simulation of quantum channels in NMR. Our approach relies on the suitable decomposition of non-unitary operators in a linear combination of d unitary ones, which can be then experimentally implemented with the assistance of a number of ancillary qubits that grows logarithmically in d . As a proof-of-principle demonstration, we realize the quantum simulation of three quantum channels for a single-qubit: phase damping (PD), amplitude damping (AD), and depolarizing (DEP) channels. For these paradigmatic cases, we measure key features, such as the fidelity of the initial state and the associated von Neuman entropy for a qubit evolving through these channels. Our experiments are carried out using nuclear spins in a liquid sample and NMR control techniques.

Introduction— In the last decades, significant progress has been achieved in the isolation and coherent control of quantum systems, allowing for the observation of their unitary dynamics [1–7]. Such a degree of controllability has resulted in the implementation of quantum machines composed of a growing number of qubits, which have been used for key tests of quantum simulations and quantum computers. As envisioned by Richard Feynman [8], large-scale quantum simulators would open the door to the analysis of new quantum physical phenomena and to the study of various models that are nowadays intractable with classical computers. In opposition to the quantum simulators of closed systems, the simulation of open quantum systems [9–12], which follow non-unitary dynamics, has been less explored. In this sense, both from a theoretical and experimental perspective, simulating open quantum systems pose relevant challenges. For example, understanding how quantum systems interact with their environment could potentially shed light on the physics of photosynthetic processes or transport phenomena in general, which in turn could help design more efficient light-harvesting devices. It could also help understand dissipation and thermalisation processes, or the nature of phase transitions. In the same manner, topics related to the foundations of quantum physics, as the measurement process or the quantum-to-classical transition, would greatly benefit from a deeper physical understanding of open quantum systems.

In this letter, we provide an efficient quantum algorithm for the implementation of non-unitary quantum dynamics associated to paradigmatic quantum channels. Our approach works by decomposing the non-unitary operators into a linear combination of unitary ones. This can be physically implemented via the assistance of a number of ancillary qubits that scales logarithmically with respect to the number of the involved unitary operators. We experimentally demonstrate our proposed quantum simulation method via the implementation

of a set of decoherence quantum channels on a nuclear spin-qubit with NMR control techniques. More specifically, we implement the phase damping (PD) channel which squashes the Bloch sphere towards a fixed axis, the amplitude damping (AD) channel which squashes the Bloch sphere towards a given state, and the depolarising (DEP) channel which acts by sending all qubit states towards the centre of the Bloch sphere.

An open quantum system can be described as the quantum dynamics of a subsystem inside a larger system which includes its environment, following the unitary transformations $\rho_{se} = U(\rho \otimes \rho_{env})U^\dagger$. Here ρ and ρ_{env} are the initial states of the system and the environment, respectively, and are considered to be initially uncorrelated. The evolution of the principal system can be retrieved as $\rho_s = \text{tr}_{env}(U(\rho \otimes \rho_{env})U^\dagger)$, where tr_{env} is the partial trace over the environment degrees of freedom [2]. Alternatively, the evolution of the system can also be described by a completely positive and trace-preserving map [13]: $\varepsilon(\rho) = \sum_k E_k \rho E_k^\dagger$, where E_k are Kraus operators satisfying $\sum_k E_k^\dagger E_k = I$. Non-unitary processes of open quantum systems can also be described by master equations. While the Kraus formalism provides the description of the dynamics for a discrete time step, a master equation can provide a continuous time evolution of the density matrix that describes the open quantum system.

Theoretical Results— Our method builds upon the framework of the so-called duality quantum computing, which was first proposed by Long [14]. Such a framework allows for the arbitrary sum of d unitary operators acting on an n -qubit system by the addition of a d -level ancillary qubit or, equivalently, $\log_2(d)$ two-level ancillary systems. Considering that Kraus operators $\{E_k\}$ can also be decomposed into a linear sum of unitary operators, duality quantum computing appears to be of direct applicability to the simulation of open quantum system. A schematics of our proposal follows these steps:

(a) A d -dimensional ancillary system is added to our working system and the setup is initialised in the quantum state $|\Psi\rangle|0\rangle$, where $|\Psi\rangle$ and $|0\rangle$ are the input states of the working system and the d -dimensional ancilla, respectively. One additional operation V is then performed on the auxiliary qubit

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$|0\rangle$, transforming the system to: $|\Psi\rangle|0\rangle \rightarrow \sum_{i=0}^{d-1} V_{i0}|\Psi\rangle|i\rangle$, where V_{i0} are the first column elements of the unitary matrix V and are determined by the target map $\{E_k\}$.

(b) The controlled operation $U_c = U_0 \otimes |0\rangle\langle 0| + U_1 \otimes |1\rangle\langle 1| + \dots + U_{d-1} \otimes |d-1\rangle\langle d-1|$ is implemented afterwards. Here, U_0, U_1, \dots, U_{d-1} are the unitary basis corresponding to the decomposition of the elements $\{E_k\}$. This will result in the system evolving to the state $\sum_{i=0}^{d-1} V_{i0}U_i|\Psi\rangle|i\rangle$.

(c) Operation W is performed on the auxiliary system, resulting in $\sum_i V_{i0}U_i|\Psi\rangle W|i\rangle = \sum_i \sum_k W_{ki}V_{i0}U_i|\Psi\rangle|k\rangle$, where U_i is unitary and $W_{ki}V_{i0}$ are complex coefficients satisfying $\sum_{i=0}^{d-1} |W_{ki}V_{i0}| \leq 1$. Thus, given a non-unitary transformation described by $\{E_k\}$, its corresponding evolution can be efficiently implemented if the unitary operations V , W , and U_c , satisfying $E_k = \sum_i W_{ki}V_{i0}U_i$, are found.

(d) Finally, measuring the corresponding final state of the working system, with the ancillary system in state $|k\rangle\langle k|$, will result in $E_k|\Psi\rangle\langle\Psi|E_k^\dagger$. Therefore, if we measure the final state of the working qubit in all the bases of the ancillary qubit, the result $\varepsilon(\rho) = \sum_k E_k\rho E_k^\dagger$, with $\rho = |\Psi\rangle\langle\Psi|$, will correspond to the simulation of the map $\{E_k\}$.

PD channel. – We will start the illustration of our method analysing the effect of a phase damping (PD) channel acting on a single-qubit [15]. The effect of the PD channel is to remove the coherences of the qubit stored in the non diagonal elements of its density matrix ρ_{in} . In the Kraus representation, this corresponds to $E_0 = [1 \ 0; 0 \ \sqrt{1-\lambda}]$ and $E_1 = [0 \ 0; 0 \ \sqrt{\lambda}]$, where the parameter $\lambda \in [0, 1]$ represents the strength of the PD channel. In Fig. 2 we give the quantum circuit that would realise such a noise channel according to the method introduced in this paper, which for this case needs the addition of a single ancillary qubit. For this case, Kraus operators E_0 and E_1 can be decomposed into a linear combination of the unitary operators \mathcal{I} and σ_z , where \mathcal{I} is a 2×2 identity matrix and $\sigma_{x,y,z}$ are Pauli matrices. The decomposition is given by $E_0 = \frac{1+\sqrt{1-\lambda}}{2}\mathcal{I} + \frac{1-\sqrt{1-\lambda}}{2}\sigma_z$ and $E_1 = \frac{\sqrt{\lambda}}{2}\mathcal{I} - \frac{\sqrt{\lambda}}{2}\sigma_z$.

It can be easily checked that the unitary operators V , W , U_0 and U_1 that fulfil conditions $E_k = \sum_{i=0}^1 W_{ki}V_{i0}U_i$ ($k = 0, 1$) for a PD channel are given by

$$U_0 = \mathcal{I}, U_1 = \sigma_z, \\ V = W = \begin{pmatrix} \sqrt{\frac{1+\sqrt{1-\lambda}}{2}} & \sqrt{\frac{1-\sqrt{1-\lambda}}{2}} \\ \sqrt{\frac{1-\sqrt{1-\lambda}}{2}} & -\sqrt{\frac{1+\sqrt{1-\lambda}}{2}} \end{pmatrix}. \quad (1)$$

As illustrated in Fig. 2, the composite system consisting of an ancillary qubit and a working qubit is initialised in state $\rho_{\text{in}}^{\text{CH}} = \rho_{\text{in}} \otimes |0\rangle\langle 0|$, with the input state of the working qubit $\rho_{\text{in}} = |\phi\rangle\langle\phi|$. In order to extract the evolution corresponding to the PD channel acting on the working qubit, we need to trace out the ancillary degrees of freedom from the final state $\rho_{\text{out}}^{\text{CH}}$. After doing so, the final state of the working qubit should correspond to $\rho_{\text{out}} = \varepsilon^{\text{PD}}(\rho_{\text{in}}) = E_0\rho_{\text{in}}E_0^\dagger + E_1\rho_{\text{in}}E_1^\dagger$. The subspace where the ancillary qubit is in the state $|0\rangle$ will be associated with the evolution of the working system that corresponds to $E_0\rho_{\text{in}}E_0^\dagger$, while the subspace of the ancilla state $|1\rangle$ will be associated to $E_1\rho_{\text{in}}E_1^\dagger$.

In order to experimentally demonstrate our proposed quantum simulation scheme, we make use of the nuclear spins in a sample of ^{13}C -labeled chloroform dissolved in deuterated acetone that we manipulate through techniques of Nuclear Magnetic Resonance (NMR) [16, 17]. The nuclear spins of ^{13}C and ^1H are used to encode the two-level working qubit and the ancillary qubit [18], respectively. We prepare the setup in a so-called pseudo-pure state (PPS) $|00\rangle\langle 00|$ starting from the thermal equilibrium state via the spatial averaging technique [19–21]. For our experimental analysis, we consider the following initial state for the working qubit: $|X\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, $|-Y\rangle = (|0\rangle - i|1\rangle)/\sqrt{2}$, and $|Z\rangle = |0\rangle$. Secondly, for each given input state ρ_{in} , we measure the expectation values $\langle\sigma_{x,y,z}\rangle = \text{Tr}(\rho_{\text{out}}\sigma_{x,y,z})$ on the working qubit at the output of the circuit, after it has undergone all the unitary steps. We do this for a collection of values of the parameter λ , ranging from 0 to 1 and incremental steps of 1/20. The output state of the working qubit ρ_{out} is directly obtained via single-qubit tomography.

The whole process, from the PPS $|00\rangle\langle 00|$ to the end of the protocol, contains the following steps: a single rotation of the system qubit to prepare its initial state $\rho_{\text{in}} \otimes |0\rangle\langle 0|$ from the PPS $|00\rangle\langle 00|$, the operations V , W , all the controlled operations, and the readout $\pi/2$ pulse. These operations are all packed up together and realised via the GRAdient Ascent Pulse Engineering (GRAPE) technique [22, 23]. The GRAPE approach provides a 5ms pulse width and over 99.5% fidelity for the whole package. Analytically, for any input state of the form $\rho_{\text{in}} = 0.5\mathcal{I} + \alpha\sigma_x + \beta\sigma_y + \gamma\sigma_z$, the PD channel should result in a final state $\rho_{\text{out}}^{\text{th}} = 0.5\mathcal{I} + \alpha\sqrt{1-\lambda}\sigma_x + \beta\sqrt{1-\lambda}\sigma_y + \gamma\sigma_z$. In our experiments, the average fidelity between the reconstructed single-qubit state $\rho_{\text{out}}^{\text{exp}}$ and the ideal output state $\rho_{\text{out}}^{\text{th}}$ is around 99.52% for all three experiments [18]. In Fig. 1(a), the expectation values of $\langle\sigma_{x,y,z}\rangle$ are plotted, which agree well with the theoretically expected values. These clearly show that the PD channel reduces all the magnetisation, $M_{x,y}$, in the xy plane, while keeping the magnetisation, M_z , in the z direction for any input state ρ_{in} .

AD channel. – We move now to analyse the case of the amplitude damping (AD) channel [24], which is characterised by taking every input state to a specific one. The AD channel is described in the Kraus representation via the operators $M_0 = [1 \ 0; 0 \ \sqrt{1-\lambda}]$ and $M_1 = [0 \ \sqrt{\lambda}; 0 \ 0]$. Alternatively, the AD change can be represented as $M_0\rho_{\text{in}}M_0^\dagger + \lambda S_0\rho_{\text{in}}S_0^\dagger$, where we have introduced matrices $S_0 = [0 \ 1; 0 \ 0]$ and $S_1 = [0 \ 0; 1 \ 0]$ for experimental convenience, which will be the effect of the AD process $\varepsilon^{\text{AD}}(\rho_{\text{in}})$. For this newly introduced Kraus operator, S_0 and S_1 , we define the operators V , W , U_0 , and U_1 of the quantum circuit in Fig. 2 to be

$$U_0 = \sigma_x, U_1 = i\sigma_y, \\ V = W = \sqrt{\frac{1}{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (2)$$

The experiment is performed in two steps, corresponding to the quantum circuit shown in Fig. 2 with two different settings of the operators V , W , U_0 , and U_1 . The first setting is chosen

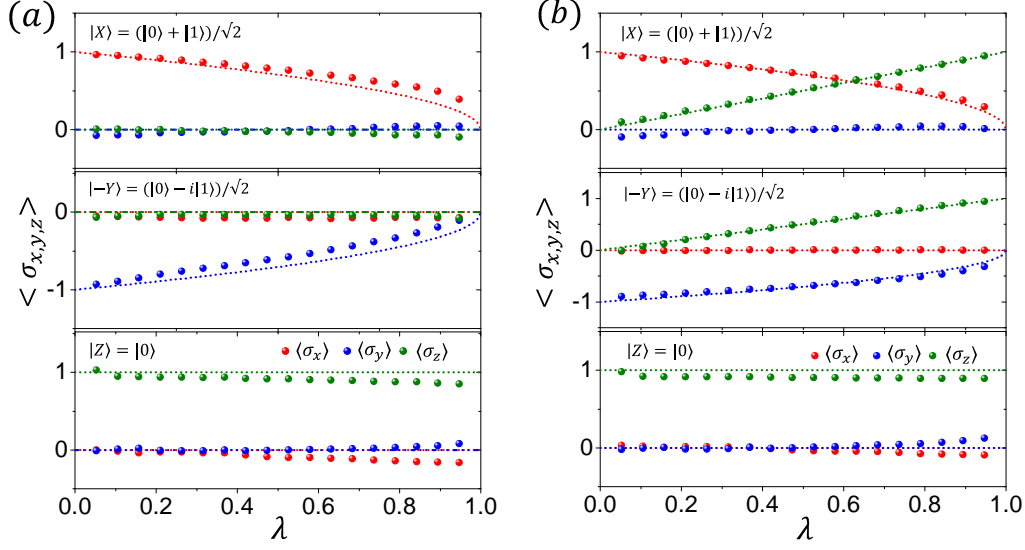


Figure 1. (a) Experimental results for the quantum simulation of the PD channel. (b) Experimental results for simulation of the AD channel. In each of the three experiments, we initially prepare the working qubit in states $|X\rangle$, $|-Y\rangle$, and $|Z\rangle$, which is easily realised by using a $\pi/2$ pulse around x axis (y axis) starting from the initial state $|Z\rangle = |0\rangle$. Then, we measure the expectation values $\sigma_{x,y,z}$ for the output state of the working qubit. The parameter λ is varied from 0 to 1 with 1/20 increments. All dots are experimental data, while the curves are the corresponding theoretical predictions.

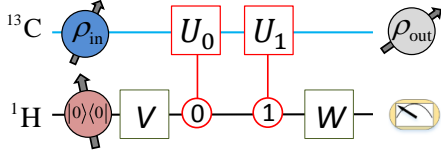


Figure 2. **Quantum circuit for the realisation of the PD (AD) channel.** The black line is the ancilla (held by the nuclear spin of ^{13}C), and the blue line is the system qubit (held by the nuclear spin of ^1H). The red blocks represent the controlled operations. Operation U_0 is applied on the second qubit if the first qubit is in the state $|0\rangle$, followed by an operator U_1 , which is applied on the second qubit if the first qubit stays in the state $|1\rangle$.

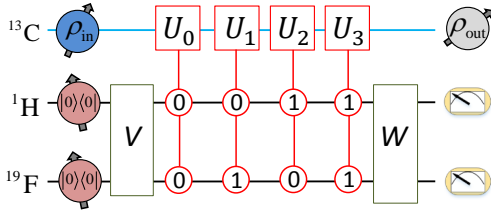


Figure 3. **Quantum circuit for realizing the DEP channel.** The black lines are the ancilla (held by the nuclear spins of ^{13}H and ^{19}F), and the blue line is the system qubit (held by the nuclear spin of ^{19}C). The red blocks represent the controlled operations, which follow the same pattern as that of Fig. (2).

according to Eq. (1), and only subspace $|0\rangle$ of the ancillary qubit is measured, which is associated to the transformation $M_0\rho_{\text{in}}M_0^\dagger$. The second setting is that shown in Eq. (2), and we only measure the subspace of the ancillary qubit corresponding to state $|0\rangle$, which leads to the term $S_0\rho_{\text{in}}S_0^\dagger$.

We use the same sample as that of the previous experiment in order to experimentally simulate the dynamics of the AD

channel. We follow the same experimental steps as those in the previous section, performing the experiment twice, for two different settings of the quantum gates in the circuit. As an example, for the case in which the expectation value $\langle\sigma_y\rangle$ of the final state is measured for the initial state $|X\rangle$, we firstly prepare the initial state $\rho_{\text{in}}^{\text{CH}} = |X\rangle\langle X| \otimes |0\rangle\langle 0|$ from the PPS and drive it following quantum circuit shown in Fig. 2, as described by Eq. (1). Then, the observable $\sigma_y \otimes |0\rangle\langle 0|$ is measured to provide the y -element associated to the evolution $M_0\rho_{\text{in}}M_0^\dagger$. Next, the same preparation and measurement are performed but this time utilizing the setting of unitary operators in Eq. (2), the results corresponding now to the y -element associated to $S_0\rho_{\text{in}}S_0^\dagger$. Combining these two results, one obtains the desired value $\langle\sigma_y\rangle$ for a qubit undergoing an AD channel. As in the previous experiment, the GRAPE technique is employed to generate the evolution corresponding to the quantum circuits. The whole sequence can be shown to have a 5ms pulse width and a 99.5% fidelity.

For the input state ρ_{in} , the AD channel can be shown to result in $\rho_{\text{out}}^{\text{th}} = 0.5\mathcal{I} + \alpha\sqrt{1-\lambda}\sigma_x + \beta\sqrt{1-\lambda}\sigma_y + (\gamma(1-\lambda) + 0.5\lambda)\sigma_z$. In Fig. 1(b), we show the experimental measurement of $\langle\sigma_{x,y,z}\rangle$, necessary for the reconstruction of the system qubit, and how these measurement compare to the analytically computed values. The experimental results show a good agreement with the theoretical predictions, with an average fidelity $F(\rho_{\text{out}}^{\text{exp}}, \rho_{\text{out}}^{\text{th}})$ that can be quantified to be around 99.87% for all three experiments. The results clearly show that the AD channel damps the system towards the ground state $|0\rangle\langle 0|$, reducing the magnetisation in the xy plane, while increasing it in the z direction. This could be of interest in the initialisation of a system that is in an arbitrary state.

We complete our analysis by the study of the behaviour of some additional properties under these quantum channels.

More precisely, we look at the fidelity $F(\rho_{\text{out}}, \rho_{\text{in}})$ and the von Neumann entropy $S(\rho_{\text{out}}) = -\text{Tr}(\rho_{\text{out}} \log_2 \rho_{\text{out}})$, for an input state $|X\rangle$ as it undergoes the PD and AD channels. These results are illustrated in Fig. (4). $F(\rho_{\text{out}}, \rho_{\text{in}})$ reflects the strength of the quantum channel acting on a qubit, which decreases for higher strength λ . $S(\rho_{\text{out}})$ quantifies the strength of the entanglement between the system qubit and the ancillary system, such that S will increase together with the strength λ of the PD channel, while will climb up and then decline for the AD channel. This happens because under the PD channel the initial state $|X\rangle$ will tend towards a maximally mixed state while, for an AD channel, it will gradually tend towards the ground state $|0\rangle$ through intermediate mixed states, respectively.

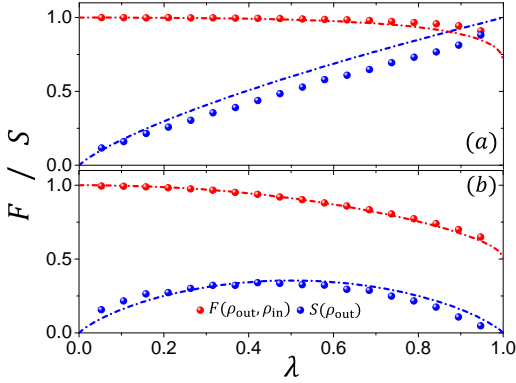


Figure 4. Fidelity $F(\rho_{\text{out}}, \rho_{\text{in}})$ and entropy $S(\rho_{\text{out}})$ for a qubit evolving under a PD channel (a), and an AD channel (b). $F(\rho_{\text{out}}, \rho_{\text{in}})$ is decreasing because the output ρ_{out} slowly deviates from the input state ρ_{in} . The behaviour of $S(\rho_{\text{out}})$ is directly guided by the entanglement strength between the system qubit and the environment, or the purity of the system qubit after tracing out the environment.

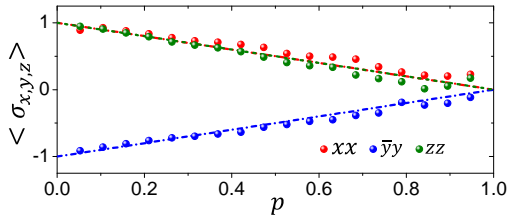


Figure 5. Experimental results for the quantum simulation the DEP channel. We perform three experiments, preparing the system qubit in state $+x$, $-y$, and $+z$, which corresponds to a direction in the Bloch sphere. We then measure the expectation value of a Pauli matrix in the same axis for each initial state. For instance, the observable $\langle \sigma_y \rangle = \text{Tr}(\rho_{\text{out}} \sigma_y)$ will be measured if the initial state is $-y$ direction. Therefore, experimental data for three different runs is presented, xx , $\bar{y}y$, and zz , as a function of parameter p . All dots are experiments, while the curves are theoretical predictions.

DEP channel. – To complete our study of decoherence channels, we consider the depolarizing (DEP) channel ε^{DEP} [25]. For this case, the Kraus representation is given by $E_0 = \sqrt{1 - \frac{3p}{4}} \mathcal{I}$, $E_1 = \sqrt{\frac{p}{4}} \sigma_x$, $E_2 = \sqrt{\frac{p}{4}} \sigma_y$, and $E_3 = \sqrt{\frac{p}{4}} \sigma_z$.

It can be trivially shown that the effect of the DEP channel on an initial state ρ_{in} is to evolve towards the maximally mixed state $\varepsilon^{\text{DEP}}(\rho_{\text{in}}) = 0.5\mathcal{I} + (1 - p)\rho_{\text{in}}$, with some probability p .

In Fig. (3), the quantum circuit to realise the quantum simulation of the DEP channel is depicted, following our proposed protocol. In this case, we set $U_0 = \mathcal{I}$, $U_1 = \sigma_x$, $U_2 = \sigma_y$, and $U_3 = \sigma_z$, while operator V is given by

$$V = \begin{pmatrix} \sqrt{1 - \frac{3p}{4}} & -\sqrt{\frac{p}{4} \frac{(1 - \frac{3p}{4})}{1 - \frac{p}{4}}} & -\sqrt{\frac{p}{4} \frac{(1 - \frac{3p}{4})}{(1 - \frac{p}{4})(1 - \frac{p}{2})}} & -\sqrt{\frac{p}{4 - 2p}} \\ \sqrt{\frac{p}{4}} & \sqrt{1 - \frac{p}{4}} & 0 & 0 \\ \sqrt{\frac{p}{4}} & -\frac{p}{4\sqrt{1 - \frac{p}{4}}} & \sqrt{\frac{1 - \frac{p}{2}}{1 - \frac{p}{4}}} & 0 \\ \sqrt{\frac{p}{4}} & -\frac{p}{4\sqrt{1 - \frac{p}{4}}} & -\frac{p}{4\sqrt{(1 - \frac{p}{4})(1 - \frac{p}{2})}} & \sqrt{\frac{4 - 3p}{4 - 2p}} \end{pmatrix}.$$

On the other hand, operation W is fixed to a 4×4 identity matrix. The quantum circuit for the DEP channel is then implemented by combining two ancillary qubits initially prepared in the state $|00\rangle\langle 00|$ and a system qubit in input state ρ_{in} . At the end of the protocol, the two ancillary qubits are traced out to acquire the output state of the DEP channel $\rho_{\text{out}} = \varepsilon^{\text{DEP}}(\rho_{\text{in}})$.

Experimentally, we need a three-qubit quantum-information processor, which is implemented via diethyl fluoromalonate dissolved in d6 acetone in NMR, where the nuclear spins of ^{13}C , ^1H , and ^{19}F in the diethyl fluoromalonate molecule act as the system qubit and the two ancillary qubits [18], respectively. The spatial averaging technique is again used to prepare the pseudo pure state $|000\rangle\langle 000|$ [26]. The unitary operators are implemented via the GRAPE technique that provides a 10ms pulse width. For the DEP channel, we only carry out xx -, $\bar{y}y$ -, and zz -experiments, which are enough to demonstrate the properties of the DEP channel. For instance, for the case of the $\bar{y}y$ -experiment, we prepare the system in the state $| - Y \rangle \langle - Y | \otimes | 00 \rangle \langle 00 |$ by applying a $\pi/2$ pulse around the x axis to the system qubit ^{13}C . Then, we measure the observable $\sigma_y \otimes \mathcal{I} \otimes \mathcal{I}$ which provides us with the expectation value $\langle \sigma_y \rangle = \text{Tr}(\rho_{\text{out}} \sigma_y)$. ρ_{out} is the output state of the system qubit ^{13}C after tracing out the ancillary qubits ^1H and ^{19}F at the end of quantum circuit. Two other experiments are performed in a similar fashion similarly corresponding to $\bar{y}y$ -experiments. Fig. (5) illustrates the corresponding results of three experiments xx , $\bar{y}y$, and zz for different values of p , which presents a good agreement between the theoretical predictions and the experiments.

Conclusion– We have proposed a method for the quantum simulation of open quantum dynamics, which grows logarithmically in the number of ancillary qubits. Moreover, we have experimentally implemented the proposed simulation procedure, realizing proof-of-principle experiments in an NMR setup. Our experiment is a small-scale demonstration of the working principles of the proposed techniques, which can be considered as building blocks for more involved protocols. The experimental results show a high degree of correspondence with the theoretical predictions, showing the capacity of our method to simulate paradigmatic decoherence channels. A natural extension of this work is the development of methods to construct algorithms to simulate the dynamics of open quantum systems in higher dimensions. For example, using the Weyl operator basis, any three-dimensional channel in the Kraus representation can be decomposed into a linear combination of Weyl operators: $M = \sum_{n,m=0}^2 b_{nm} U_{nm}$ [27],

where U_{nm} is the Weyl operator and b_{nm} are coefficients. Namely, we can perform any Kraus operator in the form a linear combination of Weyl operators with the proposed method.

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SUPPLEMENTAL MATERIAL FOR “QUANTUM SIMULATION OF QUANTUM CHANNELS IN NMR”

In this supplemental material, we provide some experimental details of the employed setup and techniques.

Experimental samples– All experiments are carried out at room temperature on a Bruker AV-400 spectrometer. The sample used for the simulation of the PD and AD channels was a liquid sample of ^{13}C -labeled chloroform dissolved in deuterated acetone. The corresponding molecule structure and parameters are illustrated in Fig. 6(a). Analogously, 6(b) shows the diethyl fluoromalonate dissolved in d_6 acetone that was used in the simulation of the DEP channel.

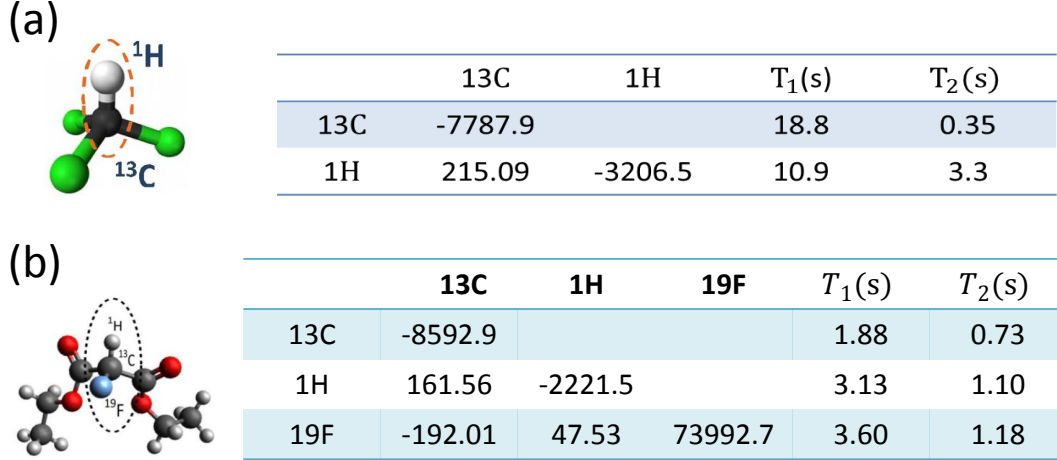


Figure 6. **Molecular structure and relevant parameters of experimental samples.** (a) ^{13}C -labeled Chloroform. (b) The diethyl fluoromalonate. The values of the chemical shifts (Hz) and J -coupling constant (Hz) between the column and row nuclei of the molecule are represented by the diagonal and off-diagonal elements of the table, respectively. The tables also provide the longitudinal time T_1 and transversal relaxation T_2 , which can be measured using the techniques such as the standard inversion recovery.

Under the weak coupling approximation, the natural Hamiltonian of an n -qubit NMR system can be expressed as

$$\mathcal{H}_{int}^n = \sum_{i=1}^n \omega_i \sigma_z^i + \sum_{i < j, i=1}^n \frac{\pi J_{ij}}{2} \sigma_z^i \sigma_z^j, \quad (3)$$

where ω_i is the chemical shift of the i th nucleus and J_{ij} is the J -coupling constant between the i th and the j th nuclear spins. Figure 6 illustrates the molecular structure and the corresponding parameters.

Initialization of the setup.– In every experiment, starting from an initial thermal equilibrium state, we first generate a pseudo-pure state (PPS) associated to the state $|0\rangle^{\otimes n}$, as the thermal state is not useful for quantum computation because it is a highly mixed state. For the employed liquid sample, the thermal equilibrium state can be written as

$$\rho_{\text{thermal}} = \frac{\mathcal{I}^{\otimes n}}{2^n} + \sum_{i=1}^n \epsilon_i \sigma_z^i, \quad (4)$$

where \mathcal{I} is a 2×2 identity matrix, n is the number of qubits, and ϵ_i represents the polarization of the i -th nucleus at room temperature. The spatial averaging technique was used to initialize our system, taking the thermal state to the following PPS

$$\rho_0 = \frac{1 - \epsilon}{2^n} \mathcal{I} + \epsilon |0\rangle\langle 0|^{\otimes n}. \quad (5)$$

A state of this form is convenient as the term related to the identity does not evolve under any unitary propagator and cannot be observed in NMR. Therefore, we can restrict our analysis to the deviation term $|0\rangle\langle 0|^{\otimes n}$ and use it to encode the behaviour of the quantum system. In the 2-qubit case, the employed pulse sequence to transfer ρ_{thermal} to ρ_0 was

$$[\alpha]_x^2 \rightarrow [G]_z \rightarrow \left[\frac{\pi}{4}\right]_{-x}^2 \rightarrow \left[\frac{1}{2J_{12}}\right] \rightarrow \left[\frac{\pi}{4}\right]_y^2 \rightarrow [G]_z, \quad (6)$$

where $\cos \alpha = 2\gamma_1/\gamma_2$, γ_1 and γ_2 being the gyromagnetic ratios, and where $[G]_z$ includes the gradient pulses that cancel all coherences of the instantaneous state.

Tracing ancillary qubits for the measurement.— For an n -qubit quantum system ρ_{SA} , with one system qubit and $(n - 1)$ ancillary qubits, the operation of tracing out the ancillary qubits, in order to obtain the state of our system qubit $\rho_S = \text{Tr}_A(\rho_{SA})$, can be realised by measuring the following operators of the output state ρ_{SA} ,

$$\mathcal{M}_{x,y,z} = \sigma_{x,y,z} \otimes \mathcal{I}^{\otimes n-1}. \quad (7)$$

In an NMR platform, 2^{n-1} peaks will be observed, with the m -th peak providing the expectation values of operators

$$\begin{aligned} \mathcal{M}_x^{m,n} &= \sigma_x \otimes |b(m-1, n-1)\rangle\langle b(m-1, n-1)| \text{ and} \\ \mathcal{M}_y^{m,n} &= \sigma_y \otimes |b(m-1, n-1)\rangle\langle b(m-1, n-1)|, \end{aligned} \quad (8)$$

where $b(m-1, n-1)$ is the binary representation of number $m-1$ in $n-1$ bits.

Summing the following results over m from 1 to 2^{n-1} leads to $\mathcal{M}_{x,y} = \sum_{m=1}^{2^{n-1}} \mathcal{M}_{x,y}^{m,n}$. To measure the observable \mathcal{M}_z , we apply an additional readout pulse ($\pi/2$ pulse around y axes) on the system qubit at the end, which transfers the magnetization in the z direction to the x direction. In this manner, the expectation value of \mathcal{M}_x corresponds the value of the desired observable \mathcal{M}_z . Moreover, single-qubit tomography of the system qubit can easily be realised using the following rule,

$$\rho_S = \frac{1}{2} \mathcal{I} + \frac{\langle \mathcal{M}_x \rangle}{2^n} \sigma_x + \frac{\langle \mathcal{M}_y \rangle}{2^n} \sigma_y + \frac{\langle \mathcal{M}_z \rangle}{2^n} \sigma_z, \quad (9)$$

where the coefficient 2^n is a normalisation constant, and $\langle \mathcal{M}_{x,y,z} \rangle$ is the expectation value of observable $\mathcal{M}_{x,y,z}$, $\text{Tr}(\rho_{SA} \mathcal{M}_{x,y,z})$.

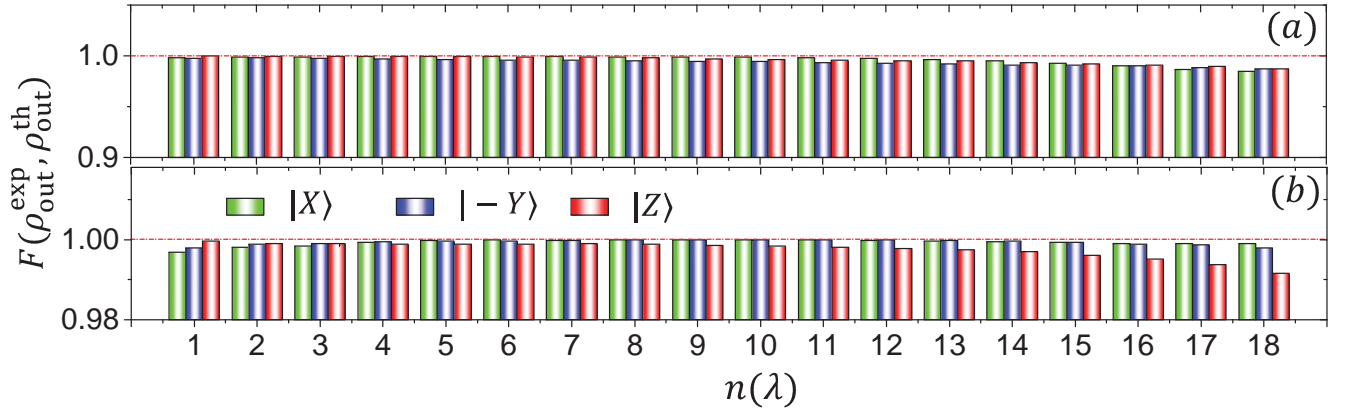


Figure 7. **Fidelity $F(\rho_{\text{out}}^{\text{exp}}, \rho_{\text{out}}^{\text{th}})$ of the state after the quantum simulation of PD and AD channel with respect to the analytically expected state.** For a number of input states $|X\rangle$, $|-Y\rangle$, and $|Z\rangle$, the output density matrices $\rho_{\text{out}}^{\text{exp}}$ are measured and their fidelity $F(\rho_{\text{out}}^{\text{exp}}, \rho_{\text{out}}^{\text{th}})$ with respect to the ideal values is computed. The subfigure (a) and (b) present the corresponding fidelities for the PD and AD channels, respectively. $n(\lambda)$ represents each of the steps of parameter λ as it increases from 0 to 1 in 18 steps.

In order to evaluate the accuracy of our simulations, we have computed the fidelity $F(\rho_{\text{out}}^{\text{exp}}, \rho_{\text{out}}^{\text{th}})$ between the reconstructed single-qubit density matrix $\rho_{\text{out}}^{\text{exp}}$ and the ideal state $\rho_{\text{out}}^{\text{th}}$ for each of the PD and AD channels. These results are illustrated in Fig. 7. The adopted fidelity definition through the whole work is $F = \text{Tr}(\rho_a \rho_b) / \sqrt{\text{Tr}(\rho_a^2) \text{Tr}(\rho_b^2)}$.